

```
% Male Mouse Liver In Vitro MCMC simulation file  
% Three chains can be run by selecting different seernd  
% and changing the output file name
```

```
prepare @clear  
prepare @all  
output @clear
```

```
VVIALF=0.01165; %% Male ==VVIAL=.0119573;  
VVIALM=0.0119573;  
VMED=.001;  
VINJF=0.0002; %% Male ==VIN=0.0003858 !important  
VINM=0.0003858 ;  
VAIRF=VVIALF-VMED;  
VAIRM=VVIALM-VMED;  
TSTOP=1.2;  
TF=0.;  
TI=0.2;  
PROT = 1.0;  
P1 = 0.69;  
WESITG=0;  
WEDITG =0;  
  
CINT = 0.1 ;  
MAXT = 0.001 ;  
TSTOP = 1.1  
  
KG1 = 0.45 ;
```

```
seedrnd(25526)  
%seedrnd(334485)  
%seedrnd(998754)
```

```
global _cal  
global _time  
global data  
global tFindex  
global tMindex  
  
global CCC  
global firstT  
global lastT  
global firstD  
global lastD  
global ControlData
```

```

use ('ControlData.m')
use ('FemaleData.m')
use ('MaleData.m')

dataF = [B6FmiceLiver(:,IDf_540ppm : IDf_10ppm)];
dataM = [B6MmiceLiver(:,IDm_529ppm : IDm_10ppm)];
data = NaN* ones([25, 10]); % correspone to max 25 timepoints and 5 dose
each gender
data(1:6, 1:5) = dataF ;
data(1:25, 6:10) = dataM;
firstT = [1, 1]
lastT = [6, 25]
firstD = [1, 6]
lastD = [5, 10]
tFindex = B6FmiceLiver(:, IDf_time);
tMindex = B6MmiceLiver(:, IDm_time);

AA=dataF(1,:)*(VAIRF+P1*VMED);
BB=dataM(1,:)*(VAIRM+P1*VMED);
CCC = [AA, BB];
data = log(data);

function preds = getpreds(Vmax, Km, VK, A10, Gender)
global _ca1
global _time
global tFindex
global tMindex
global ControlData

% draw back ground loss rate
tmp = ceil(rand*500);
lossR = ControlData(tmp);

setmdl("VMAX1", exp(Vmax)); % reset model parameter as global
variables
setmdl("KM1", exp(Km));
setmdl("VK", VK);
setmdl("A10", A10);
setmdl("RLOSS", exp(lossR));

if Gender==1
    tindex = tFindex;
    setmdl ("VVIAL", 0.01165);
    setmdl ("VINJ", 0.0002);
else
    tindex = tMindex;
    setmdl ("VVIAL", 0.0119573);
    setmdl ("VINJ", 0.0003858);
end

data @clear

```

```
data("SAMPTIMES", ["T"], tindex);

start @nocallback

preds = NaN*ones(length(tindex), 1);

for i = 1:length(tindex)
    idx = find(_time == tindex(i));
    if(idx ~= [])
        preds(i) = max(0.0, _cal(idx));
    end
end

preds = log(preds);

use ".\MCMCscripts\mminvitrolivl1v1.m"

chains = runmcmc();

save @file=mmouseleverredol.dat @format=ascii @separator=tab chains
```